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Preferential protonation and methylation site of thiopyrimidine derivatives in solution: NMR data

Kozlov A., Semenov V., Mikhailov A., Aganov A., Smith M., Reznik V., Latypov S.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Protonation (alkylation) sites of several thiopyrimidine derivatives were directly determined by 1H-15N (1H- 13C) heteronuclear single quantum coherence/heteronuclear multiple bond correlation methods, and it was found that in all compounds, protonation (methylation) occurred at the N1 nitrogen. GIAO DFT chemical shifts were in full agreement with the determined tautomeric structures. According to ab initio calculations, the stability of the different protonated forms and methylated derivatives was favored due to thermodynamic control and not kinetic control. © 2008 American Chemical Society.

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